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SIMULATION OF DROPLET COALESCE USING
LATTICE BOLTZMANN METHOD

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SUPERVISOR'S DECLARATION

I hereby declare that I have checked this project and in my opinion, this project is adequate in terms of scope and quality for the award of the degree of Bachelor of Mechanical Engineering.

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STUDENT'S DECLARATION

I hereby declare that the work in this project is my own except for quotations and summaries which have been duly acknowledged. The project has not been accepted for any degree and is not concurrently submitted for award of other degree.

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Dedicate to my beloved dad, mom and my honour siblings

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ABSTRACT

In this project, a single component multiphase (SCMP) LBM is proposed to simulate the phenomenon of droplet coalesce using Lattice Boltzmann method. The basic idea is to see on how two stationary droplet without collision will merge together. Besides, effect of the height on droplet's neck or interface is studied in this thesis. A development on Lattice Boltzmann method is storied from early where it is evolved by Lattice Gas approach and it is continue with the Navier-Stokes equation and collision theory. A derivation of the Lattice Boltzmann scheme from the classical Boltzmann equation is dicussed in detail. According to the problems, a single component multiphase (SCMP) LBM is used or involved in the equation in order to solve more phase of fluids. Before that, investigation on non ideal fluid is discussed using van der Waals fluids where the critical constant of pressure, volume and temperature is solved. By doing this, it will tell the characteristic of the liquid and gas phase. From the Maxwell equal area construction, the value of macroscopic variables, density of fluids is determined which will be code in the algorithm. Algorithm of multiphase LBM involving the initial condition, streaming step, collision step and boundary condition is coded to done the simulation. The progress of droplet coalesce will occur from initial until steady state. The study on droplet coalesce proven where the neck height of droplets will increase as the time step increased. The two droplets will merge together until steady state and become one big droplet.

ABSTRAK

Dalam projek ini, satu komponen multi fasa diusulkan untuk simulasi fenomena penggabungan titisan menggunakan kaedah Lattice Boltzmann. Idea asalnya adalah untuk melihat bagaimana dua titisan pegun tanpa pelanggaran akan bercantum bersama. Selain itu, kesan pada tinggi leher titisan atau permukaan dalam yang bercantum dikaji dalam tesis ini. Perkembangan mengenai kaedah Lattice Boltzmann diceritakan daripada awal yang mana ia bermula daripada pendekatan Lattice Gas dan ia berterusan dengan melibatkan persamaan Navier-Stokes dan teori pelanggaran. Penciptaan skim Lattice Boltzmann daripada persamaan klasik Boltzmann dibincangkan dengan terperinci. Berdasarkan masalah, satu komponen multi fasa digunakan atau dilibatkan dalam persamaan yang mana untuk menyelesaikan bendalir yang mempunyai lebih fasa. Sebelum itu, penyiasatan terhadap bendalir tidak ideal dibincangkan menggunakan teori bendalir van der Waals di mana pemalar kritikal untuk tekanan, isipadu dan suhu diselesaikan. Dengan melakukan ini, ia dapat memberitahu perwatakan untuk fasa cecair dan gas. Daripada pembinaan luas sama Maxwell, nilai untuk perkara makroskopik iaitu ketumpatan bendalir boleh diperolehi dan dikodkan di dalam algoritma. Algoritma multi fasa kaedah Lattice Boltzmann melibatkan keadaan awal, langkah pergerakan, langkah pelanggaran dan keadaan sempadan dikodkan untuk menghasilkan simulasi. Perjalanan dalam penggabungan titisan akan berlaku daripada awal sehingga keadaan stabil. Kajian terhadap penggabungan titisan dibuktikan dimana tinggi leher titisan akan meningkat sebagaimana masa meningkat. Dua titisan tersebut akan bercantum sehingga stabil dan menjadi satu titisan besar.

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LIST OF SYMBOLS

a	Acceleration
	Constant/Characteristic of individual gas
b	Constant/Characteristic of individual gas
\mathbf{c}	Micro velocity vector
c_s	Speed of sound
$f(x, c, t)$	Density distribution function
f_i	Discretised density distribution function
$f_{\mathbf{c}i}^{\mathbf{eq}}$	Discretised equilibrium density distribution function
g	Particle's relative velocity
n	Number of moles
P	Pressure
P_c	Critical Pressure
P_{LG}	Liquid-gas Pressure
R	Gas constant ($0.0821 \text{ L atm mol}^{-1}\text{K}^{-1}$)
t	Time
T	Temperature
T_c	Critical Temperature
u	Velocity
V	Volume
V_c	Critical Volume

V_L	Liquid volume
V_G	Gas Volume
α	Sign for component of vector
β	Sign for component of vector
σ	Scattering cross section
ρ	Macroscopic density
τ	Time relaxation
ν	Viscosity
Ω	Collision operator

LIST OF ABBREVIATIONS

CFD	Computational Fluid Dynamics
LBM	Lattice Boltzmann method
PDE	Partial Differential equation
LBE	Lattice Boltzmann equation
LGA	Lattice Gas Approach
BGK	Bhatnagar-Gross-Krook
D2Q9	Two dimensionals nine velocities model
FYP	Final year project
FE	Free Energy
SCMP	Single Component Multiphase
vs	Versus

CHAPTER 1

INTRODUCTION

1.1 PROJECT BACKGROUND

Understanding the science of fluid dynamics is important in many branches of engineering. It is also broad, interdisciplinary field that touches almost every aspect of our daily lives. Fluid dynamics involving aerospace, automotive, chemical processing, power generation, heating, ventilation, air conditioning, biomedical, oil and gas, marine and many others.

Nowadays, there is a lot of research and investigation about the flow dynamics behavior. With the recent advances in computing power today's microprocessor, numerical investigation and solutions of flow problems can be brought to the desktop. Because fluid related problems arising in science and engineering are extremely complex by nature, the use of a computer is necessary to determine the fluid motion of a particular problem.

There are many type of computational method in order to solve fluid flow problem and it is becomes a very important tools to researcher. According to fluid flow phenomenon, the computational fluid dynamics (CFD) is one of the branches of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. In order to that, Lattice Boltzmann method (LBM) is introduced which is one class of computational fluid dynamics method for fluid simulation.

1.2 COMPUTATIONAL FLUID DYNAMICS (CFD)

Computational fluid dynamics (CFD) has grown from a mathematical curiosity to become an essential tool in solving the Navier-Stokes equation and the continuity equation or an equation derived from them. In other words, CFD is the science of determining a numerical solution to the governing equations of fluid flow while advancing the solution through space or time to obtain a numerical description of the complete flow field of interest.

The basic of this CFD is represented by a partial differential equation (PDE) widely known as the incompressible Navier-Stokes equation. Solving this equation is a very challenging task to exactly simulate fluid flow on a computer. A lot of numerical method was introduced by mathematicians and engineers in CFD, such as Finite Difference Method, Finite Element Method and Finite Volume Method to solve the Navier-Stokes equation numerically.

The classical approach in CFD, treat of such fluids and describe the new physical properties in terms of transport phenomena are related to a new observable, macroscopic property. A PDE is written down for the dynamics of this property then is solved by an appropriate numerical technique. In a fluid with important temperature variations for example, a new observable property, the temperature, is introduced and its dynamics is described by a heat transport equation.

1.3 LATTICE BOLTZMANN METHOD (LBM)

Lattice Boltzmann methods (LBM) is a class of computational fluid dynamics (CFD) methods for fluid simulation. Instead of solving the Navier–Stokes equations, the discrete Boltzmann equation is solved to simulate the flow of a Newtonian fluid with collision models such as Bhatnagar-Gross-Krook (BGK). By simulating the interaction of a limited number of particles the viscous flow behavior emerges automatically from the intrinsic particle streaming and collision processes.

Although LBM approach treats gases and liquids as system consisting of individual particles, the primary goal of this approach is to build a bridge between the microscopic and macroscopic dynamics, rather than to deal with macroscopic dynamics directly. In other words, the goal is to derive macroscopic equations from microscopic dynamics by means of statistic, rather than to solve macroscopic equations.

The LBM has a number of advantages over other conventional CFD methods. The algorithm is simple and can be implemented with a kernel of just a few hundred lines. The algorithm can also be easily modified to allow for the application of other, more complex simulation components. For example the LBM can be extended to describe the evolution of binary fluid, or extended to allow for more complex boundary conditions. Thus the LBM is an ideal tool in fluid simulation.

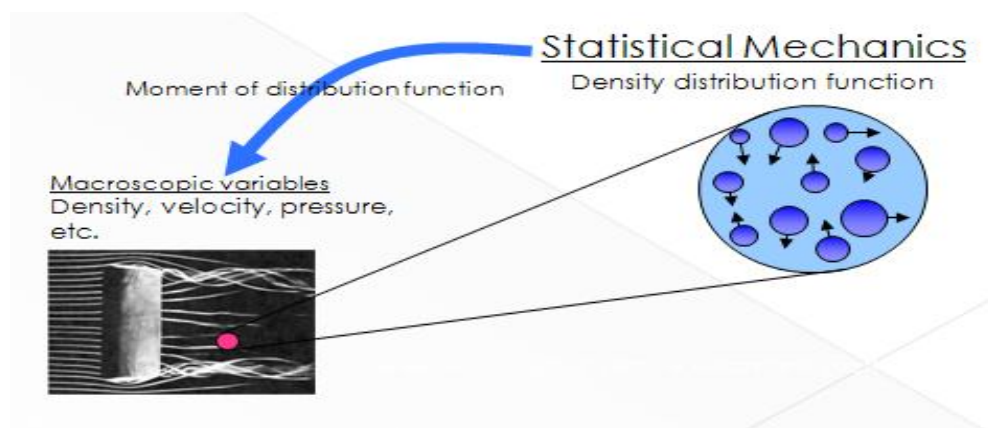


Figure 1.1: General concept of Lattice Boltzmann method

1.4 PROBLEM STATEMENT

Conventional CFD methods not able to models the fluid consisting of fictive or small particles, and such particles perform consecutive propagation and collision processes over a discrete lattice mesh. It is also lack in dealing with complex boundaries, incorporating of microscopic interactions and parallelization of the algorithm. For multiphase flow, it is a complicated physical phenomenon to be solved using CFD where two or more phases coexist (with gas-solid, gas-liquid, liquid-liquid, being the simplest combinations).

1.5 OBJECTIVE

To simulate 2-Dimensional droplet coalesce using Lattice Boltzmann method.

1.6 SCOPES

In order to achieve the objectives notified earlier, the following scopes have been recognized:

- 1) Literature of lattice Boltzmann method.
- 2) Understand the theory of lattice Boltzmann method.
- 3) Use Free Energy (FE) parameters proposed by Nik Mohd Izual [12].
- 4) Simulate the phenomenon of droplet coalesce.

CHAPTER 2

LITERATURE REVIEW

2.1 INTRODUCTION

In the last few years, we have witnessed a rapid development of the method known as the lattice Boltzmann equation (LBE). Although only in its infancy, the LBE method has demonstrated its ability to simulate hydrodynamic systems, chemicals reactive flow, single component multiphase fluid system and multi component multiphase fluid flow. Together with modern computers of massively parallel processors, the LBE method has become a powerful computational method for studying various complex systems.

The lattice Boltzmann equation can be directly derived from the continuous Boltzmann equation discretized in some special manner in both time and phase space. Some analysis shows that theoretically the lattice Boltzmann equation is independent of the lattice gas automata. The lattice Boltzmann equation is a finite difference form of the continuous Boltzmann equation. We provide a detailed account of an a priori derivation of the lattice Boltzmann equation from its continuous counterpart, the continuous Boltzmann equation. A general procedure to derive lattice Boltzmann models from the continuous Boltzmann equation is established.

2.2 LATTICE GAS APPROACH

An alternative approach to these computational fluid dynamics simulations was invented in the late 1980s with the lattice gas methods. These methods allowed particles to move on a discrete lattice and local collisions conserved mass and momentum [1]. Because the continuity and Navier Stokes equations are only continuous forms of the mass and momentum conservation statements and method that locally conserves mass and momentum will obey some kind of continuity and Navier Stokes equations and it was shown that the lattice gas methods could be used to simulate (rather noisy) hydrodynamics. However, the lattice gas methods had several drawbacks consisting mainly of their noisy nature and the appearance of some additional terms in the Navier Stokes level equations that limited their success. It was then discovered that instead of discrete particles a density distribution could be advecting which eliminated the noisyness of the method and allowed for a more general collision operator.

The time evolution of the LGA consists of a collision step and a propagation step. In the collision step, particles can change their velocities' direction due to collisions and in the propagation step, particles move in the direction of their velocities to the new sites where they will collide again. The collision rules are chosen in order to conserve both mass and momentum. The detailed nature of the microscopic interactions does not affect the form of the equations but only the values of the coefficients (such as the viscosity) appearing in them.

To summarize, LGA are inherently simple, their discrete nature makes them straight forward to implement by computer and they lend themselves to agent based approaches which reflect the intrinsic individuality of cells. Local rules can be developed from a microscopic level phenomenon understanding which is direct and intuitive. LGA provide an opportunity to study interactions and behavior which are difficult to formulate as continuum equations [2].

2.3 NAVIER-STOKES EQUATION

The mathematical relationship governing fluid flow is the famous continuity equation and Navier-Stokes equation given by:

$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} \quad (2.1)$$

With velocity \mathbf{u} , density ρ , and kinematics shear viscosity ν . The Navier-Stokes equation is a nonlinear partial differential equations [3] and so complex that there is currently no analytical solution to them except for a small number of special cases.

Kinematics shear viscosity ν is

$$\frac{2\tau - 1}{6} \quad (2.2)$$

Solving this we can obtain time relaxation τ ,

$$3\nu + \frac{1}{2} \quad (2.3)$$

2.4 CLASSICAL BOLTZMANN EQUATION

The lattice Boltzmann method (LBM) was originally developed as a natural extension to the gas automata for modeling fluid flow based upon kinetic theory. As a new computational fluid dynamics (CFD) tool, the method has received considerable attention in recent years. Much progress has been made during the last few years that extends the LBM as a tool for simulating a number of complex problems, especially some flows which are quite difficult to simulate using conventional method [4].

Lattice Boltzmann equation is directly obtained from the lattice gas automata by taking ensemble average with the assumption of random phase, leading to the following equation [5] ;

$$f(x + c\Delta t, t + \Delta t) - f(x, t) = \Omega(f) \quad (2.4)$$

Where $f(x, c, t)$ is the single particle distribution function with discrete velocity c . $\Omega(f)$ is the lattice Boltzmann collision operator.

Distribution function $f(x, c, t)$ describes the number of particles at position x , move with velocity c at time t . Two conditions are related to the distribution function; one without collisions and one with collisions.

At a short time Δt , each particle moves from x to $x + c\Delta t$ and each particle velocity changes from c to $c + a\Delta t$, where a is the acceleration due to external forces on a particle at x with a velocity c . Hence, the number of molecules $f(x, c, t)dxdc$ is equal to the number of molecules $f(x + c\Delta t, c + a\Delta t, t + \Delta t)dxdc$, for the distribution without collisions [6]. Therefore;

$$f(x + c\Delta t, c + a\Delta t, t + \Delta t)dxdc - f(x, c, t)dxdc = 0 \quad (2.5)$$

There will be a net difference between the number of molecules $f(x, c, t)dxdc$ and the number of molecules $f(x + c\Delta t, c + a\Delta t, t + \Delta t)dxdc$ if collision occurs between the molecules. This can be expressed by;

$$f(x + c\Delta t, c + a\Delta t, t + \Delta t)dxdc - f(x, c, t)dxdc = \Omega_a(f)dxdc\Delta t \quad (2.6)$$

where $\Omega(f)dxdc\Delta t$ is the collision operator. On dividing by cdt , and letting dt tends to zero ($dt \sim 0$) give the Boltzmann equation for f

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial c_\alpha} + a \frac{\partial f}{\partial c_\alpha} = \Omega(f) \quad (2.7)$$

2.5 BOLTZMANN COLLISION FUNCTION

Any solution of the Boltzmann equation, requires that an expression for the collision operator $\Omega(f)$. If the collision is to conserve mass, momentum and energy, it is required that

$$\int \begin{bmatrix} 1 \\ c \\ c^2 \end{bmatrix} \Omega(f) dx \quad (2.8)$$

Collision can change the distribution function $f(x,c,t)$ in two ways;

1. Some particle originally having velocities c will have some different velocity after the collision. This cause a decrease in $f(x,c,t)$.
2. Some particles have other velocities may have the velocity c a collision, increasing $f(x,c,t)$.

The form of the collision can be found [7] by assuming that:

- Only binary collisions need to be considered (dilute gas)
- The influence of container walls may be neglected
- The influence of the external force (if any) on the rate of collisions is negligible
- Velocity and position of a uncorrelated (assumption of molecular chaos)

Suppose two particles with initial velocities c and c_1 have velocities c' and c_1' after a collisions. Since all particles have the same mass, conservation of momentum and energy require that

$$c + c_1 = c' + c_1' \quad (2.9)$$

$$\frac{1}{2} |c|^2 + \frac{1}{2} |c_1|^2 = \frac{1}{2} |c'|^2 + \frac{1}{2} |c_1'|^2 \quad (2.10)$$

$$|\mathbf{c} + \mathbf{c}_1| = |\mathbf{c}' + \mathbf{c}_1'| \quad (2.11)$$

Under all these assumptions, the Boltzmann equation takes on the following form:

$$\Omega(f) = \iint (ff_1 - f'f'_1)g\sigma d\Omega dc' \quad (2.12)$$

Where: $f(x, c, t)$, $f_1(x, c_1, t)$, $f'(x, c', t)$, $f'_1(x, c'_1, t)$, g is the particles relative velocity before the collision and σ is the scattering cross section.

2.6 BHATNAGAR-GROSS-KROOK (BGK) COLLISION MODEL

The Boltzmann equation was derived earlier for a gas consisting of hard-sphere molecules and undergoing binary collisions. It describes the evolution of the distribution function on a lattice in a manner that macroscopic fluid dynamical behavior is recovered. The fluid density, momentum and energy can then be found from the distribution function by considering the appropriate integral. However, one of the major problems when dealing with the Boltzmann equation is the complicated nature of the collision integral. Any replacement of collision must satisfy the conservation of mass, momentum, and energy by Eq.(2.8). The idea behind this replacement is that the large amount of detail of two-body interactions is not likely to influence significantly the values of many experimental measured quantities.

Recall the Boltzmann equation without external force

$$\frac{\partial f}{\partial t} + \mathbf{c}_a \frac{\partial f}{\partial \mathbf{x}} = \left. \frac{\partial f}{\partial t} \right|_{\text{collision}} \quad (2.13)$$

Where,

$$\left. \frac{\partial f}{\partial t} \right|_{\text{collision}} = \Omega(f) \quad (2.14)$$